

Dr. Volodymyr Farafonov
curriculum vitae



➤ **Personal data**

Other names: Vladimir S. Farafonov
Date of birth: 10 November 1992
Nationality: Ukraine

➤ **Contact information**

Job address: Department of Physical Chemistry, School of Chemistry,
V. N. Karazin Kharkiv National University, 4 Svoboda sq., Kharkiv, 61022, Ukraine
Job phone: (057) 707 54 45
Cell phone: (095) 318 92 45
Job e-mail: farafonov@karazin.ua

➤ **Education**

18.12.2018: Ph.D. degree awarded for the thesis «Localization and hydration of organic dyes in surfactant micelles by molecular dynamics simulations» (specialty «Physical chemistry», code 02.00.04)
11.2014 – 03.2018: Ph.D. student at the Department of Physical Chemistry, School of Chemistry, V.N. Karazin Kharkiv National University (KhNU)
09.2009 – 06.2014: Undergraduate student at the School of Chemistry, KhNU

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➤ **Employment**

01.2024 – <i>present</i>	Senior Research Fellow	Department of Physical Chemistry, KhNU
01.2020 – 12.2022		
01.2018 – 01.2020	Research Fellow	<i>same place</i>
09.2019 – <i>present</i>	Assistant Professor	<i>same place</i>
04.2018 – 09.2019	Teacher	<i>same place</i>
05.2018 – <i>present</i>	Visiting Research Fellow	School of Engineering and Applied Science, Aston University, Birmingham, UK
10.2017 – 01.2018	Research Associate	<i>same place</i>
03.2017 – 05.2017	Engineer	Research Institute of Chemistry, KhNU
03.2016 – 06.2016	Junior Research Fellow	Department of Physical Chemistry, KhNU

➤ **Research interests**

— Investigation of micellar solutions with molecular dynamics
— Computer simulations of biomolecules, in particular, viruses
— Participation in development of multiscale molecular dynamics/fluctuating hydrodynamics method

➤ Honours and awards

- Award of Kharkiv regional state administration in regard to the Day of Science in Ukraine in 2023
- Winner of the district stage of the municipal competition «Young person of the year — 2020» in nomination «Scientific activity» in Kharkiv city
- Laureate of the Award of Supreme Council of Ukraine for young scientists in 2019 as a member of a collective for the work „Complex ecological approach to design of novel functional materials for chemical analysis and technology”
- Associate member of the Royal Society of Chemistry from 2016, membership number 620846

➤ Publications

- h-index 11 (Scopus profile <https://www.scopus.com/authid/detail.uri?authorId=56717430500>)
- 40 articles, including 25 Scopus-cited
- 24 conference papers, including 14 papers for international conferences
ORCID: <https://orcid.org/0000-0003-0785-9582>

Selected articles in Scopus-cited journals:

1. **Farafonov, V. S.**; Stich, M.; Nerukh, D. A. Complete Virion Simulated: All-Atom Model of an MS2 Bacteriophage with Native Genome. *J. Chem. Theory Comput.* **2023**. DOI: <https://doi.org/10.1021/acs.jctc.3c00846>
2. Vodolazkaya, N.; Laguta, A.; **Farafonov, V.**; Nikolskaya, M.; Balklava, Z.; Khayat, R.; Stich, M.; Mchedlov-Petrosyan, N.; Nerukh, D. Influence of various colloidal surfactants on the stability of MS2 bacteriophage suspension and charge distribution of PCV2 virus surface. *J. Mol. Liq.* **2023**, 387, 122644. DOI: [10.1016/j.molliq.2023.122644](https://doi.org/10.1016/j.molliq.2023.122644)
3. **Farafonov, V. S.**; Lebed, A. V.; Nerukh, D. A.; Mchedlov-Petrosyan, N. O. Estimation of Nanoparticle’s Surface Electrostatic Potential in Solution Using Acid-Base Molecular Probes I: *In silico* Implementation for Surfactant Micelles. *J. Phys. Chem. B.* **2023**, 127(4), 1022–1030. DOI: [10.1021/acs.jpcc.2c07012](https://doi.org/10.1021/acs.jpcc.2c07012)
4. **Farafonov, V. S.**; Lebed, A. V.; Nerukh, D. A.; Mchedlov-Petrosyan, N. O. Estimation of nanoparticle’s surface electrostatic potential in solution using acid-base molecular probes II: Insight from atomistic simulations of micelles. *J. Phys. Chem. B.* **2023**, 127(4), 1031–1038. DOI: [10.1021/acs.jpcc.2c07028](https://doi.org/10.1021/acs.jpcc.2c07028)
5. **Farafonov, V. S.**; Stich, M.; Nerukh, D. Reconstruction and validation of entire virus model with complete genome from mixed resolution cryo-EM density. *Faraday Discuss.* **2022** Advance Article. DOI: [10.1039/D2FD00053A](https://doi.org/10.1039/D2FD00053A)
6. Abdelhalim, A. O. E.; Sharoyko, V. V.; Ageev, S. V.; **Farafonov, V. S.**; Nerukh, D. A.; Postnov, V. N.; Petrov, A. V.; Semenov, K. N. Graphene Oxide of Extra High Oxidation: A Wafer for Loading Guest Molecules. *J. Phys. Chem. Lett.* **2021**, 12(41), 10015–10024. DOI: [10.1021/acs.jpcclett.1c02766](https://doi.org/10.1021/acs.jpcclett.1c02766)
7. Li, F.; Korotkin, I.; **Farafonov, V.**; Karabasov, S. Lateral migration of peptides in transversely sheared flows in water: An atomistic-scale-resolving simulation. *J. Mol. Liq.* **2021**, 337, 116111. DOI: [10.1016/j.molliq.2021.116111](https://doi.org/10.1016/j.molliq.2021.116111)
8. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Computing pK_a Shifts Using Traditional Molecular Dynamics: Example of Acid–Base Indicator Dyes in Organized Solutions. *J. Chem. Theory Comput.* **2020**, 16(9), 5852–5865. DOI: [10.1021/acs.jctc.0c00231](https://doi.org/10.1021/acs.jctc.0c00231)

9. **Farafonov, V. S.**, Nerukh, D. MS2 bacteriophage capsid studied using all-atom molecular dynamics. *Int. Focus* **2019**, *9*(3), 20180081. DOI: [10.1098/rsfs.2018.0081](https://doi.org/10.1098/rsfs.2018.0081)
10. Tarasova, E.; **Farafonov, V.**; Taiji, M.; Nerukh, D. Details of charge distribution in stable viral capsid. *J. Mol. Liq.* **2018**, *265*, 585–591. DOI: [10.1016/j.molliq.2018.06.019](https://doi.org/10.1016/j.molliq.2018.06.019)
11. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Character of localization and microenvironment of solvatochromic Reichardt's betaine dye in sodium *n*-dodecyl sulfate and cetyltrimethylammonium bromide micelles: molecular dynamics simulation study. *Langmuir* **2017**, *33*(33), 8342–8352. DOI: [10.1021/acs.langmuir.7b01737](https://doi.org/10.1021/acs.langmuir.7b01737)
12. **Farafonov, V. S.**; Lebed, A. V. Developing and validating a set of all-atom potential models for sodium dodecyl sulfate. *J. Chem. Theory Comput.* **2017**, *13*(6), 2742–2750. DOI: [10.1021/acs.jctc.7b00181](https://doi.org/10.1021/acs.jctc.7b00181)
13. Tarasova, E.; **Farafonov, V.**; Khayat, R.; Okimoto, N.; Komatsu, T.; Taiji, M.; Nerukh, D. All-atom molecular dynamics simulations of entire virus capsid reveal the role of ion distribution in capsid's stability. *J. Phys. Chem. Lett.* **2017**, *8*(4), 779–784. DOI: [10.1021/acs.jpcllett.6b02759](https://doi.org/10.1021/acs.jpcllett.6b02759)
14. Tarasova, E.; Korotkin, I.; **Farafonov, V.**; Karabasov, S.; Nerukh, D. Complete virus capsid at all-atom resolution: Simulations using molecular dynamics and hybrid molecular dynamics/hydrodynamics methods reveal semipermeable membrane function. *J. Mol. Liq.* **2017**, *245*(Supplement C), 109–114. DOI: [10.1016/j.molliq.2017.06.124](https://doi.org/10.1016/j.molliq.2017.06.124)
15. Korotkin, I.; Nerukh, D.; Tarasova, E.; **Farafonov, V.**; Karabasov, S. Two-phase flow analogy as an effective boundary condition for modelling liquids at atomistic resolution. *J. Comput. Sci.* **2016**, *17*(part 2), 446–456. DOI: [10.1016/j.jocs.2016.03.012](https://doi.org/10.1016/j.jocs.2016.03.012)

Other articles in Scopus-cited journals:

1. Tariq, S.S.; Zia, K.; Nur-e-Alam, M.; Nerukh, D.; **Farafonov, V. S.**; Ul-Haq, Z. Impact of mutations in SARS-CoV-2 recombinant sub-variant XBB.1.16 on the binding affinity with human ACE2 receptor. *J. Mol. Graph. Model.* **2024**, *131*, 108813. DOI: [10.1016/j.jmgm.2024.108813](https://doi.org/10.1016/j.jmgm.2024.108813)
2. Vodolazkaya, N.; Nikolskaya, M.; Laguta, A.; **Farafonov, V.**; Balklava, Z.; Stich, M.; Mchedlov-Petrosyan, N.; Nerukh, D. Estimation of nanoparticle's surface electrostatic potential in solution using acid-base molecular probes. III: Experimental hydrophobicity/hydrophilicity and charge distribution of MS2 virus surface. *J. Phys. Chem. B.* **2022**, *126*(41), 8166–8176. DOI: [10.1021/acs.jpccb.2c04491](https://doi.org/10.1021/acs.jpccb.2c04491)
3. Maximova, E.; Postnikov, E. B.; Lavrova, A. I.; **Farafonov, V.**; Nerukh, D. Protein-Ligand Dissociation Rate Constant from All-Atom Simulation. *J. Phys. Chem. Lett.* **2021**, *12*(43), 10631–10636. DOI: [10.1021/acs.jpcllett.1c02952](https://doi.org/10.1021/acs.jpcllett.1c02952)
4. Sharoyko, V.; Iamalova, N. R.; Ageev, S. V.; Meshcheriakov, A. A.; Iurev, G. O.; Petrov, A. V.; Nerukh, D. A.; **Farafonov, V. S.**; Vasina, L. V.; Penkova, A. V.; Semenov, K. N. *In Vitro* and *In Silico* Investigation of Water-Soluble Fullerenol C₆₀(OH)₂₄: Bioactivity and Biocompatibility. *J. Phys. Chem. B* **2021**, *125*(32), 9197–9212. DOI: [10.1021/acs.jpccb.1c03332](https://doi.org/10.1021/acs.jpccb.1c03332)
5. Wu, Y.; Okesola, B. O.; Xu, J.; Korotkin, I.; Berardo, A.; Corridori, I.; di Brocchetti, F. L. P.; Kanczler, J.; Feng, J.; Li, W.; Shi, Y.; **Farafonov, V.**; Wang, Y.; Thompson, R. F.; Titirici, M.-M.; Nerukh, D.; Karabasov, S.; Oreffo, R. O. C.; Rodriguez-Cabello, J. C.; Vozi, G.; Azevedo, H. S.; Pugno, N. M.; Wang, W.; Mata, A. Disordered protein-graphene oxide co-assembly and supramolecular biofabrication of functional fluidic devices. *Nat. Commun.*, **2020**, *11*, 1182. DOI: [10.1038/s41467-020-14716-z](https://doi.org/10.1038/s41467-020-14716-z)
6. Vus, K.; Tarabara, U.; Balklava, Z.; Nerukh, D.; Stich, M.; Laguta, A.; Vodolazkaya, N.; Mchedlov-Petrosyan, N. O.; **Farafonov, V.**; Kriklya, N.; Gorbenko, G.; Trusova, V.; Zhytniakivska, O.; Kurutose, A.; Gadjev, N.; Deligeorgiev, T. Association of novel monomethine cyanine dyes with bacteriophage MS2: A fluorescence study. *J. Mol. Liq.* **2020**, *302*, 112569. DOI: [10.1016/j.molliq.2020.112569](https://doi.org/10.1016/j.molliq.2020.112569)

7. Mchedlov-Petrosyan, N. O.; **Farafonov, V. S.**; Cheipesh, T. A.; Shekhovtsov, S. V.; Nerukh, D. A.; Lebed, A. V. In search of an optimal acid-base indicator for examining surfactant micelles: Spectrophotometric studies and molecular dynamics simulations. *Colloids Surf., A* **2019**, *565*, 97–107. DOI: [10.1016/j.colsurfa.2018.12.048](https://doi.org/10.1016/j.colsurfa.2018.12.048)
8. Mchedlov-Petrosyan, N. O.; **Farafonov, V. S.**; Lebed, A. V. Examining surfactant micelles via acid-base indicators: Revisiting the pioneering Hartley-Roe 1940 study by molecular dynamics modeling. *J. Mol. Liq.* **2018**, *264*, 683–690. DOI: [10.1016/j.molliq.2018.05.076](https://doi.org/10.1016/j.molliq.2018.05.076)
9. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Solvatochromic betaine dyes of different hydrophobicity in ionic surfactant micelles: Molecular dynamics modeling of location character. *Colloids Surf., A* **2018**, *538*, 583–592. DOI: [10.1016/j.colsurfa.2017.11.046](https://doi.org/10.1016/j.colsurfa.2017.11.046)
10. Korotkin, I.; Karabasov, S.; Nerukh, D.; Markesteijn, A.; Scukins, A.; **Farafonov, V.**; Pavlov, E. A hybrid molecular dynamics/fluctuating hydrodynamics method for modelling liquids at multiple scales in space and time. *J. Chem. Phys.* **2015**, *143*, 014110. DOI: [10.1063/1.4923011](https://doi.org/10.1063/1.4923011)

Articles in local journals:

1. **Farafonov, V. S.** Computing ionization free energies of indicator dyes in micelles with fast growth alchemical transformation. *Kharkiv University Bulletin. Chemical Series.* **2024**, *42* (65), 45–52. DOI: [10.26565/2220-637X-2024-42-05](https://doi.org/10.26565/2220-637X-2024-42-05)
2. Bakumenko, M.; Bardik, V.; **Farafonov, V.**; Nerukh, D. The Multiscale hybrid method with a localized constraint: II. Hybrid equations of motion based on variational principles. *Ukr. J. Phys.* **2024**, *69*(4), 269–277. DOI: [10.15407/ujpe69.4.269](https://doi.org/10.15407/ujpe69.4.269)
3. Mchedlov-Petrosyan, N. O.; **Farafonov, V. S.**; Lebed, A. V. Solvatochromic and acid-base molecular probes in surfactant micelles: Comparison of molecular dynamics simulation with the experiment. *Liquids* **2023**, *3*, 314–370. DOI: [10.3390/liquids3030021](https://doi.org/10.3390/liquids3030021).
4. Kharchenko, D. V.; **Farafonov, V. S.**; Cheipesh, T. O.; Mchedlov-Petrosyan, N. O.; Rodik, R. V.; Kalchenko, V. I. Catalytic properties of calixarene bearing choline groups in the processes of ester hydrolysis. *Theor. Exp. Chem.* **2022**, *58*(5), 363–371. DOI: [10.1007/s11237-023-09752-x](https://doi.org/10.1007/s11237-023-09752-x)
5. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Localization of Hydrophobized Coumarin and Xanthene Acid-Base Indicators in Micelles. *Theor. Exp. Chem.* **2022**, *58*(3), 181–189. DOI: [10.1007/s11237-022-09734-5](https://doi.org/10.1007/s11237-022-09734-5)
6. Kononenko I. V., **Farafonov, V. S.** Examination of mixed sodium dodecyl sulfate – 1-butanol micelles with molecular dynamics. *Kharkov Univ. Bull., Chem. Ser.* **2022**, *38*(61), 16–22. DOI: [10.26565/2220-637X-2022-38-02](https://doi.org/10.26565/2220-637X-2022-38-02)
7. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Continuum electrostatics investigation of ionic micelles using atomistic models. *Ukr. Chem. J.* **2021**, *6*(87), 55–69. DOI: [10.33609/2708-129X.87.06.2021.55-69](https://doi.org/10.33609/2708-129X.87.06.2021.55-69)
8. **Farafonov, V. S.**; Lebed, A. V. Nitroxyl spin probe in ionic micelles: A molecular dynamics study. *Kharkov Univ. Bull., Chem. Ser.* **2020**, *34*(57), 57–64. DOI: [10.26565/2220-637X-2020-34-02](https://doi.org/10.26565/2220-637X-2020-34-02)
9. Tkachenko, V. V.; **Farafonov, V. S.**; Tokarev, V. V.; Tkachenko, I. G. Study of the effectiveness of various cannabinoid receptor 1 (CB1) agonists using molecular docking and molecular dynamics modeling. *Fr.-Ukr. J. Chem.* **2020**, *8*(1), 76–87. DOI: [10.17721/fujcV8I1P76-87](https://doi.org/10.17721/fujcV8I1P76-87)
10. **Farafonov, V. S.**; Lebed, A. V.; Khimenko, N. L.; Mchedlov-Petrosyan, N. O. Molecular dynamics study of an acid-base indicator dye in Triton X-100 non-ionic micelles. *Voprosy Khimii i Khimicheskoi Tekhnologii* **2020**, *1*, 97–103. DOI: [10.32434/0321-4095-2020-128-1-97-103](https://doi.org/10.32434/0321-4095-2020-128-1-97-103)

11. Tarasova, E.; **Farafonov, V.**; Nerukh, D. Molecular dynamics study of the role of ions in maintaining virus capsid stability. *Ensemble* **2019**, *21*(1), 50–54. DOI: [10.11436/mssj.21.50](https://doi.org/10.11436/mssj.21.50)
12. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. An MD simulation study of Reichardt's betaines in surfactant micelles: unlike orientation and solvation of cationic, zwitterionic, and anionic dye species within the pseudophase. *Kharkov Univ. Bull., Chem. Ser.* **2018**, *30*(53), 27–35. DOI: [10.26565/2220-637X-2018-30-03](https://doi.org/10.26565/2220-637X-2018-30-03)
13. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Examining solvatochromic Reichardt's dye in cationic micelles of different size via molecular dynamics. *Voprosy Khimii i Khimicheskoi Tekhnologii* **2018**, *5*, 62–68. <http://vhht.dp.ua/wp-content/uploads/pdf/2018/5/Farafonov.pdf>
14. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Solvatochromic Reichardt's dye in micelles of sodium cetyl sulfate: MD modeling of location character and hydration. *Kharkov Univ. Bull., Chem. Ser.* **2017**, *28*(51), 5–11. DOI: [10.26565/2220-637X-2017-28-01](https://doi.org/10.26565/2220-637X-2017-28-01)
15. **Farafonov, V. S.**; Lebed, A. V. Molecular dynamics simulation study of cetylpyridinium chloride and cetyltrimethylammonium bromide micelles. *Kharkov University Bull., Chem. Ser.* **2016**, *27*(50), 25–30. DOI: [10.26565/2220-637X-2017-27-03](https://doi.org/10.26565/2220-637X-2017-27-03)
16. **Farafonov, V. S.**; Lebed, A. V. Molecular dynamics study of tetrapropylammonium ion localization in micellar solution of sodium dodecyl sulfate (in Russian). *Kharkov University Bull., Chem. Ser.* **2016**, *26*(49), 73–79. DOI: [10.26565/2220-637X-2017-26-08](https://doi.org/10.26565/2220-637X-2017-26-08)

Selected conference papers:

1. Bakumenko, M.; Bardik, V.; **Farafonov, V.**; Nerukh, D. Multiscale Hybrid Model for Liquids: Coupling Molecular Dynamics with Hydrodynamics in Simulations. EMLG-JMLG 2024 annual meeting, 8-13 September 2024, Trieste, Italy, **2024**.
2. **Farafonov, V.S.**; Bakumenko, M., Yanushevskiy, A.; Bardik, V.; Pozhilenkov, A.; Kalachev, A.; Vaysfeld, N.; Stich, M.; Nerukh, D. All-atom MD of entire virus with genome in solution at physiological conditions. WATOC 2020, 12th Triennial Congress of the World Association of Theoretical and Computational Chemists, Vancouver, Canada, **2022**.
3. **Farafonov, V. S.**; Vodolazkaya, N.; Nikolskaya, M.; Laguta, A.; Balklava, Z.; Stich, M.; Mchedlov-Petrosyan, N.; Dmitry Nerukh, D. All-atom structure and dynamics of entire virus with genome in solution at physiological conditions. Faraday joint interest group conference (online), **2021**.
4. Vodolazkaya, N.; Nikolskaya, M.; Laguta, A.; **Farafonov, V.**; Balklava, Z.; Stich, M.; Mchedlov-Petrosyan, N.; Nerukh, D. Experimentally measured hydrophobicity and charge distribution on MS2 virus surface. Joint EMLG/JMLG Annual Meeting, 8-13 September 2019, Kutna Hora, Czech Republik, **2019**.
5. **Farafonov, V. S.**; Mchedlov-Petrosyan, N. O.; Lebed, A. V. Locus and local environment of two dyes in surfactant micelles from molecular dynamics simulations. Physics of Liquid Matter: Modern Problems: 8th International conference: Abstracts, 18-22 May 2018, Kyiv, Ukraine, **2018**.
6. **Farafonov, V. S.**; Lebed, A. V.; Mchedlov-Petrosyan, N. O. Molecular dynamics study of locus of the standard Reichardt's indicator in ionic micelles. IXth International chemistry conference "Kyiv-Toulouse" dedicated to the 100th anniversary of Fedir Babichev: Materials of reports and performances, 4-9 June 2017, Kyiv, Ukraine, **2017**.
7. Nerukh, D.; Karabasov S.; Tarasova, E.; Korotkin, I.; **Farafonov, V.**; Plyusnov, D.; Vaysfeld, N. Hybrid Molecular Dynamics - hydrodynamics modelling of liquidsolutions: whole virus at atomistic resolution. Joint EMLG/JMLG Annual Meeting, 10-14 September 2017, Vienna, Austria, **2017**.
8. **Farafonov, V. S.**; Nerukh, D. A.; Tarasova, E. A. Microscopic conditions in a virus capsid at molecular level. Physics for Life Sciences: I Russian conference, 12-16 September 2016, Saint Petersburg, Russia, **2016**.

9. Karabasov, S.; Korotkin, I.; Nerukh, D.; Tarasova, E.; **Farafonov, V.**; Markesteijn, A. Hybrid modelling based on two-phase flow analogy: advances and challenges. Hybrid Simulation Methods in Fluid Dynamics: Models, Software and Applications, Munich, Germany, **2015**.
10. Nerukh, D.; Karabasov, S.; Scukins, A.; Pavlov, E.; Korotkin, I.; **Farafonov, V.**; Taiji, M. Hybrid molecular dynamics–hydrodynamics framework for modelling liquid molecular systems: EMLG - JMLG annual meeting, 7-12 September 2014, Rome, Italy, **2014**.
11. **Farafonov, V. S.**; Lebed, A. V. Using molecular dynamics simulation for interpretation of Raman spectra of acetonitrile solution of sodium iodide. Karazin Chemistry Readings – 2014: VI All-Ukrainian scientific conference, 22-24 April 2014, Kharkiv, Ukraine, **2014**.

➤ **Computer skills**

Operating systems: advanced knowledge of Microsoft Windows; experience of Linux (including compilation and installation of software)

Desktop software: advanced knowledge of Microsoft Office, graphics editors

Scientific software: advanced knowledge of GROMACS, VMD, Origin; experience of GAMESS/FireFly, Gaussian, APBS, AIMPack, MathCAD.

Programming languages: advanced knowledge of C, Pascal/Delphi, AWK, Bash; experience of C#, TCL.

➤ **Language skills**

Ukrainian, Russian (native languages), English (level B2)

➤ **Referees**

Head of Department: Prof. Nikolay Mchedlov-Petrosyan

Department of Physical Chemistry, School of Chemistry, V.N. Karazin Kharkiv National University, Svobody sq. 4, Kharkiv, 61022, Ukraine

Phone: +38 (057) 707 5266, e-mail: nikolay.mchedlov@gmail.com

Ph.D. co-supervisor: Dr. Dmitry Nerukh

Department of Mathematics, Aston University, Aston Triangle, Birmingham, B4 7ET, UK

Phone: +44 (0) 121 204 3533, e-mail: d.nerukh@aston.ac.uk

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